COUPLING OF ATOMISTIC AND CONTINUUM SIMULATIONS USING A BRIDGING SCALE DECOMPOSITION*

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Molecular dynamics (MD) simulations have become prominent as a useful tool for gaining insight into complex physical phenomena in solids, such as fracture, surface friction, and plasticity. However, the length and time scales that can be probed using MD are still fairly limited. One possible approach to solving realistic problems is to use MD only in localized regions in which the atomic-scale dynamics are important, and a continuum simulation method (such as finite elements) everywhere else. However, most existing techniques for coupling the two simulations require that the coarse scale mesh be graded down to the atomic lattice scale at the boundary between the continuum and MD domains, so that finite element nodes coincide with atoms. The result is a very fine element mesh near the boundary region.

We present a new method for coupling molecular dynamics and continuum mechanics simulations that is based on the projection of the MD solution onto coarse scale shape functions. This projection, or "bridging scale", represents that part of the solution that is obtainable by both the MD and continuum solution methods. By subtracting the bridging scale from the total solution, we arrive at a coarse-fine decomposition that, by a proper choice of project operator, decouples the kinetic energy of the two simulations. The resulting decomposition can be used in a dynamic, finite-temperature simulation method in which MD is used only in a localized region, while the continuum simulation covers the entire domain, including the MD region to which it is coupled. This method does not require that the coarse scale mesh be graded down to the atomic lattice spacing at the boundary of the MD region. Another major advantage of this approach is that separate time step sizes can be used in the two simulations, so that the coarse scale time step is not limited to the time scale of the atomic vibrations present in the fine scale.

A known difficulty with dynamic coupling of MD and continuum simulations is the treatment of boundary conditions at the limits of the MD domain. If done improperly, small scale waves originating in the MD solution cannot pass into the coarse scale region, and are reflected at the boundary back into the MD region. In the bridging scale coupling method, the proper MD boundary condition can be derived by eliminating analytically the fine scale degrees of freedom that are not represented by the coarse scale. The resulting force boundary condition has the expected form of a generalized Langevin equation, including a time-history integral that properly dissipates the small scale energy. It is shown through several simple examples that this boundary condition gives the correct transfer of energy out of the MD region. Finally, a straighforward method for computing the kernel function for the time-history integral for 2D and 3D periodic crystal structures is presented. This method is demonstrated for carbon lattices in the graphene and diamond configurations.

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